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1. REPORT DATE *(DD-MM-YYYY)* 30May 2001	2. REPORT TYPE Final	3. DATES COVERED *(From - To)* 1Dec99-30 Nov00

4. TITLE AND SUBTITLE	
Combustion Coupled Flow Dynamics in Solid Rocket Motors	5a. CONTRACT NUMBER
	5b. GRANT NUMBER F49620-00-1-0175
	5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)	
	5d. PROJECT NUMBER
	5e. TASK NUMBER
D. R. Kassoy	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Colorado at Boulder Mechanical Engineering Department 427 UCB Boulder CO. 80309-0427	8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NA 801 N. Randollph St., Rm. 732 Arlington, VA. 22203	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

Unlimited: approved for public release

13. SUPPLEMENTARY NOTES

14. ABSTRACT The literature on pulse detonation engine (PDE) and pulse detonation rocket engine (PDRE) modeling and experiments has been reviewed with the goal of determining characteristic operational time and length scales, key parameter ranges and approaches used for evaluating device efficiency. The roles of igniter power level, duration and location on the initiation of a detonation has been assessed for gaseous mixture systems and those based on multi-phase sprays.

A secondary phase of the project is focused on the completion of technical papers describing the nonlinear dynamics of unstable solid rocket motors. Results from nonlinear asymptotic analysis and computation predict the initiation of the acoustic disturbances, the role they play in the generation of vorticity and thermal gradients, as well as the further evolution of these disturbances. Results are valid for pressure disturbances as large as 10% of the base value, relative to those from linear stability theories, where disturbances must be a factor of 100 smaller

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON D. R. Kassoy
a. REPORT	b. ABSTRACT	c. THIS PAGE			
Unclassified	unclassified	unclassified	Unlimited	38	19b. TELEPHONE NUMBER *(Include area code)* 303 492-6066

COMBUSTION-COUPLED FLOW DYNAMICS IN SOLID ROCKET MOTORS

Grant No. F49620-00-1-0175

Final Technical Report
1 December 1999 to 30 November 2000

prepared for

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May 30, 2001

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c. M. Rempe, P. L. Staab and D. R. Kassoy, "Thermal Response for an Internal Flow in a Cylinder with Time Dependent Sidewall Mass Addition", AIAA 2000-0996, 38th Aerospace Sciences Meeting, Reno, NV., (2000)

d. P. L. Staab and D. R. Kassoy, "Three Dimensional Flow in a Cylinder with Sidewall Mass Addition", submitted to Physics of Fluids, (2000)

e. K. Kirkkopru, D. R. Kassoy, Q. Zhao and Peter Staab, "Acoustically Generated Unsteady Vorticity Field in a Long, Narrow Cylinder with Sidewall Injection", submitted to the J. of Engineering Mathematics, (2000)

f. A. K. Hegab and D. R. Kassoy, "The Thermal Response of an Internal Flow in an SRM Chamber Model", AIAA 2001-0338, 39th Aerospace Science Meeting, Reno, NV., (2001)

g. A. K. Hegab and D. R. Kassoy, "Internal Flow Temperature Dynamics in a Channel with Time-dependent Mass Injection" submitted to J. Propulsion and Power, (2001)

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    a. Jennifer Russell, "An Introduction to Detonation Waves and Pulse Detonation Engines" Independent Study Final Report, Mechanical Engineering Department, University of Colorado, May 1, 2000

    b. Tanarit Sakulyanontvittaya, "Literature Review of Experiments Involving Detonations in Liquid Fuel Spray/Oxidizer Mixtures", Final Report for MCEN 5208, Introduction to Research, Mechanical Engineering Department, University of Colorado, May 1, 2001

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[1] Title page and/or Abstract only-manuscripts are available upon request.

1. ABSTRACT

The literature on pulse detonation engine (PDE) and pulse detonation rocket engine (PDRE) modeling and experiments has been reviewed with the goal of determining characteristic operational time and length scales, key parameter ranges and approaches used for evaluating device efficiency. The roles of igniter power level, duration and location on the initiation of a detonation has been assessed for gaseous mixture systems and those based on multi-phase sprays.

A secondary phase of the project is focused on the completion of technical papers describing the dynamics of co-existing irrotational and rotational disturbances in models of unstable solid rocket motors. Intense, transient vorticity and thermal gradients, generated on the chamber sidewall from inviscid, non-conducting interactions between the flow dynamics and the fluid injected from the surface, are described. Both nonlinear asymptotic analysis and computation are used to predict the initiation of the acoustic disturbances, the role they play in the generation of vorticity and thermal gradients, as well as the evolution of these disturbances with the passage of time. These results, valid for pressure disturbances as large as 10% of the base value supplement those from more traditional linear stability theories, where disturbances must be a factor of 100 smaller

2. PROJECT OBJECTIVES, STATUS AND ACCOMPLISHMENTS

This one-year project had both a primary and secondary objective. The former involved the development of a modeling capability for the thermal initiation and subsequent evolution of detonation waves in the pulsed detonation engine (PDE) and pulse detonation rocket engine (PDRE) environments. Literature surveys were used to assess the state of PDE/PDRE development, including theory and experiment, and to identify the characteristics of detonation initiation and evolution in liquid fuel spray/gaseous oxidizer mixtures. Concurrently, computational results were obtained for the deflagration-to-detonation transition (DDT) caused by rapid, localized thermal power deposition into a reactive gas mixture.

The second objective was to complete several manuscripts describing transient flow dynamics that occur in nearly isothermal. but thermally active models of a solid rocket motor (SRM) chamber. The results provide new perspectives about the velocity, pressure and temperature phenomena occurring in these systems. Their application to the design process should foster the development of more reliable motors with predictable performance. Publications listed in Section 5 are available upon request.

2a. Primary Objective-PDE/PDRE   Detonation   Modeling

A detonation processes reactive material on an extremely short time scale, relative to that of a typical flame used in most practical propulsion devices. The rapid chemical heat release is associated with elevated pressure levels arising from nearly constant volume heat addition, resulting in a compressive, high-speed lead shock wave system. Numerous efforts have been made to use the released energy and high pressure in

propulsion devices (see Ref. 1 for an extensive review). During the last decade interest has focused on pulsed detonation engines.

The basic concept of a PDE is relatively simple. First, an injected fuel/oxidizer mixture fills a substantial fraction of the cylindrical chamber. The pulse of mass injection from the endwall is the source of an initiation shock running through the hot gaseous products of reaction from the previous cycle. When the shock exits the PDE chamber a backward running expansion wave helps to purge some of the remaining gaseous products. Meanwhile, the unreacted mixture interface (perhaps preceded by a layer of inert buffer gas) moves down the chamber at approximately the mass input speed. The combustion process is initiated at or near the endwall well before the expansion wave front reaches the forward moving interface in order to sustain the pressure of the fresh mixture and to avoid the loss of unburned reactant across the PDE exit.

The outcome of a combustion initiation process is sensitive to igniter location, duration and power deposition. If the igniter is effective, a detonation is achieved a short distance downstream of the igniter. The initial high pressure, the source of thrust in a PDE, is relieved subsequently by backward moving rarefaction waves behind the detonation that reduce the axial speed to zero on the endwall.

Just after the detonation leaves the PDE, a new set of expansion waves are created at the exit. These help to purge the burnt products of reaction and lower the chamber pressure as they run back toward the endwall. Another cycle is started when the endwall pressure reaches a relative minimum.

Although the PDE concept is easy to understand, a variety of impediments have made practical operation a challenge (see Refs. 2 and 3 for early reviews of progress). Technical problems to be addressed include;

1. combustion initiation reliability (e.g. fuel/oxidizer mixing, time-scales for breakup and vaporization of low volatility hydrocarbon fuel droplets (see Refs. 4-7)),
2. "deflagration-to-detonation" (DDT) transition lengths (8),
3. effective removal of burned gas products,
4. thermal losses to the chamber sidewall,
5. suppression of autoignition at the fresh mixture-burned gas interface,

These problems affect both traditional PDEs and those designed for rocket applications (PDREs) described in Ref. 9. Various engineering "fixes" have been used to overcome the combustion difficulties including turbulence-generating devices (e.g., Schelkin spirals(10)) that enhance mixing and reaction rates in order to promote more sustainable reactant burning and reduce DDT lengths. They may also enhance thermal losses to the chamber walls.

While gaseous fuel/oxidizer PDEs have been the primary focus of attention, others have developed devices operating on multiphase reactant mixtures composed of low volatility liquid fuels and either oxygen or air. Brophy et. al. (11) and Brophy and Netzer (12) have demonstrated low frequency operation with JP-10 and oxygen, although

experiments with air were not successful. This genre of reactant system is important because it may more practical to use liquid fuels in PDE applications.

Operational evaluation of PDEs is usually expressed in terms of specific impulse (see Ref. 13 for an extensive review). There continues to be considerable controversy in the literature about the range and maximum values obtainable. The result depends on the pressure time-history on the endwall (thrust plate) during each cycle of the PDE. Li et. al, (14) show that predictions from modeling depend intimately on the boundary conditions used at the PDE chamber exit. In particular, inappropriate modeling of the backward moving rarefaction waves created when the detonation exits the chamber lead to inaccurate estimates of the endwall pressure time-history and hence to erroneous measures of time averaged thrust and specific impulse.

Most models of detonation phenomena in PDE's and detonation tubes are designed to predict chamber travel times and pressure-time histories (e.g., Refs. 13-19). Combustion initiation is often facilitated by imposing a blast wave of specified magnitude on the reactive mixture (16, 17 and 20) or by using an induction time model (14). Normally, scant attention is given to the details of the initiation process itself. Rather, the primary goal is to produce a sustained detonation as quickly as possible, follow its evolution through the unburned mixture in the chamber and then the sequence of chamber pressure relaxation processes caused by the backward moving rarefactions referred to earlier. This approach anticipates that the detonation formation process is relatively independent of the igniter characteristics. However, it is likely that the early time history of a combustion wave initiated by an imposed shock (e.g, Refs. 16 and 20) will differ considerably from that following spark ignition or a related form of thermal excitation. This difference can be important in PDE applications where the DDT length needs to be minimized. It may also affect impulse estimates because the initiator power input can be the source of a substantial portion of the elevated pressure at the endwall (13).

Mathematical models of thermally initiated planar detonations have been developed in the past to study the earliest phases of combustion wave formation. Numerical solutions to the complete, reactive Navier-Stokes equations (21, 22) are used to show that a significant heat transfer rate from a hot boundary to a colder reactive gas, initially at rest, can be the source of a complex initiation process on the $O(\mu s)$ time-scale.

Refs. 23 and 24 describe a more physically versatile model of detonation initiation and evolution following thermal power deposition (e.g, a spark) directly into a specified volume of reactive gas at rest adjacent to an insulated boundary. Reactive Euler equations are solved computationally to describe the birth of an overdriven detonation and its evolution to a C. J. wave. A nondimensional equation system is used to describe exothermic reactive gasdynamics occurring on a range of times scales greater the molecular collision time and less than O(1ms.), the latter being characteristic of a detonation travel time in a 1m. tube. Time-dependent spatial distributions of pressure, density, temperature, fuel concentration and velocity are analyzed to characterize the transient wave development process. The earliest phase of the initiation process is composed of a sequence of localized, transient exothermic "explosions" occurring at isolated locations behind a relatively weak lead shock. Each of the reaction centers or

hot spots is the source of strong compression waves that propagate both forward toward the lead shock and backward toward the endwall. Forward moving waves steepen and evolve into new shocks that coalesce with the lead wave to produce a stronger initial jump in the thermodynamic variables. The resulting large temperature rise is sufficient to initiate a new combustion zone directly behind the shock. Meanwhile, the retrograde compression waves also steepen and create new shocks that ignite unburned pockets of reactants left behind by the original lead shock. A new set of compression waves is generated by the rapid reaction transients in the localized "pockets". Those moving forward further enhance the strength of the lead combustion wave, enabling it to make a rapid transition into an overdriven detonation. An example, given in Ref. 23, predicts a DDT in a length of 1.36cm and a time of 2×10^{-5}s. for a reasonable set of chemico-physical parameters and a volumetric power deposition of $O(10^{11}W/m^3)$. Related results appear in Ref. 35.

Explosive transients predicted by the computational model are planar analogues of the "explosions within explosions" observed by Oppenheim and co-workers (25). Related transient events and associated pressure spikes are also seen in two-phase detonation initiation in low-volatility fuel droplet sprays (5, 11,12, 26 and 27).

Sequenced, rapid exothermic transients, occurring at discrete locations in a reactive mixture, appear to characterize detonation initiation and evolution in traditional detonation tube environments. It is expected that similar events will occur in the PDE environment, subsequent to the filling process. An understanding of short-time combustion transients may help designers to identify system parameters (e.g, igniter location, power deposition level, power deposition timing, reactant characteristics, endwall geometry) that characterize reliable, repetitive controlled initiation.

Detonation Initiation Concepts

The reliability of cyclic PDE operation and the specific impulse obtained (13), are sensitive to the time-history of the detonation initiation process associated with a specific ignition device. Typically, a high pressure and temperature driver, or even a short detontation tube is employed as an initiator (18-20, 28). The energy levels required for successful detonation generation tend to be device-related. Observations and predictions from experiments and modeling imply that a substantial portion of the endwall pressure rise results from the power deposition by the initiator, rather than from the detonation itself. Since operational PDEs are more likely to employ a thermal igniter (a spark plug, for example), rather than some form of blast wave generator, it would helpful to focus attention on the role of localized, rapid power deposition directly into the reactive material. The goal is to ascertain the system parameters to which the initiation process is most sensitive.

Recent computational results by Kuehn et. al. (24) confirm earlier conclusions (23) that a detonation does not arise directly from the initial high speed deflagration created by thermal power deposition. Rather, it appears after a sequence of compression waves, generated by isolated power bursts from exploding hot spots, coalesce into a very strong lead shock. An example of these transients in shown in Figs. 1-6 (copies of annotated transparencies from technical presentations).

The nondimensional spatial temperature distribution in Fig. 1 is given for a sequence of four nondimensional times. A high temperature, rightward moving high-speed deflagration appears adjacent to the boundary, the result of thermal power deposition at an earlier time. Subsequent expansion of the hot gases has generated a lead shock seen to the right. An exploding reaction center can be observed at some distance behind the shock. To the left of the hot spot there is a pocket of relatively cold, unburned reactant. Later, in Fig. 2, there is a new shock to right of the expanding hot spot, generated by the relaxation of the high pressure spot observed in Fig. 3 for the same time period. Fig. 4 shows that shock coalescence creates yet another localized reaction zone, coupled to the strengthened lead shock. Additional supporting compression waves are generated in this region of rapid and large heat release. Finally, an over-driven detonation, seen in Fig. 5, appears at a well defined downstream location (the DDT distance), propagates to right and eventually relaxes to a C.J wave for the reactant model used. In this time regime, the unburned pocket of gas is actually moving back toward wall due to passage of a sequence of retrograde pressure waves generated by the localized hot spots described earlier.

Global heat release as a function of time is shown in Fig. 6. One should note the relative level and duration of;
1. the initial thermal power deposition,
6. the early heat release from the high speed deflagration,
7. the period of minimal chemical heat release,
8. the subsequent rapid and variable increase in global heat release, leading to a maximal power burst when the reaction behind the shock is initiated, and even
9. the late pulse when the unburned pocket is finally consumed.

The modeling in (24) is based on a nondimensional form of the reactive Euler equations with one-step Arrhenius kinetics:
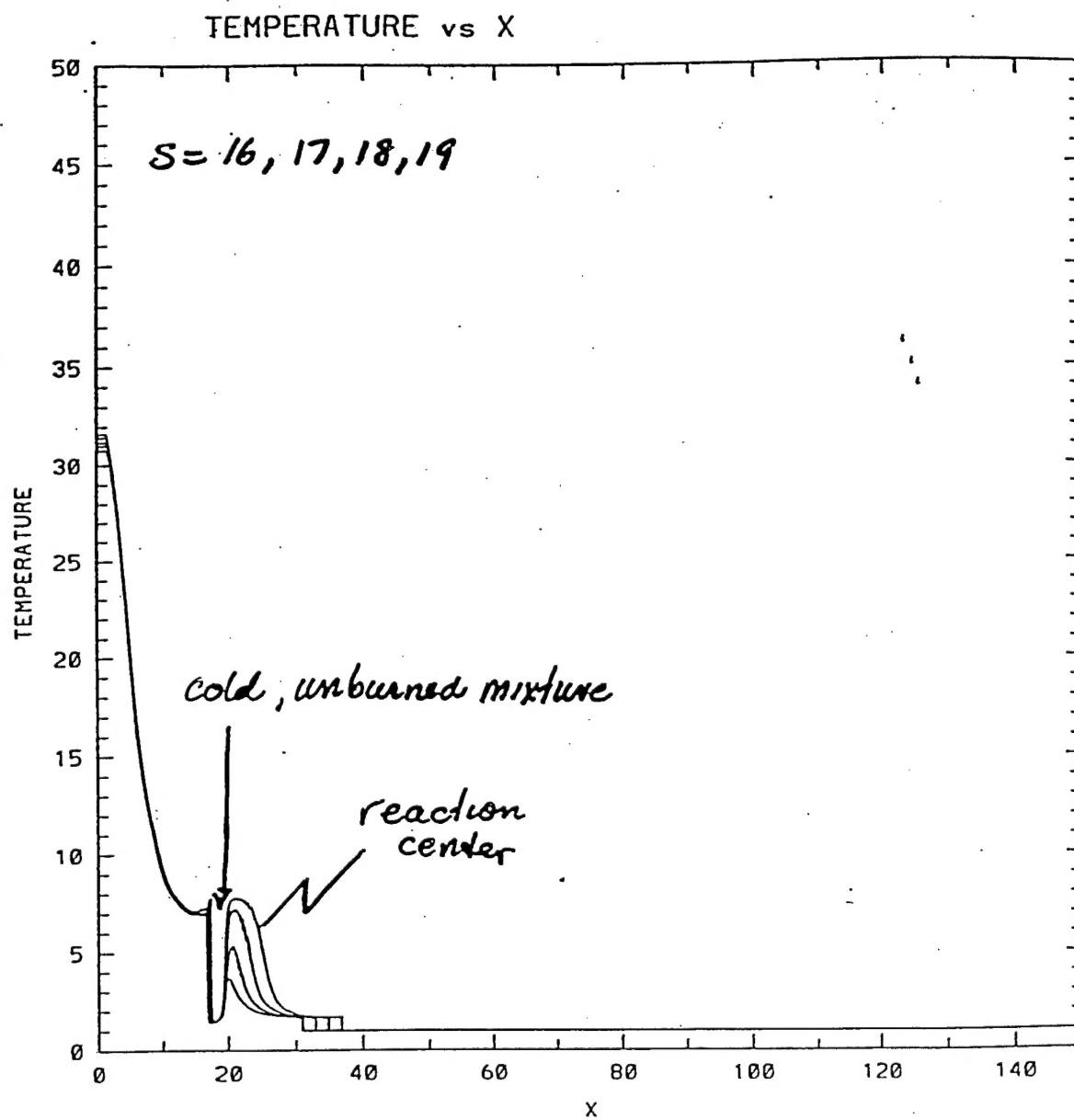
$$p = \rho T \quad , \tag{1}$$

$$\rho_t + (\rho u)_x = 0 \quad , \tag{2}$$
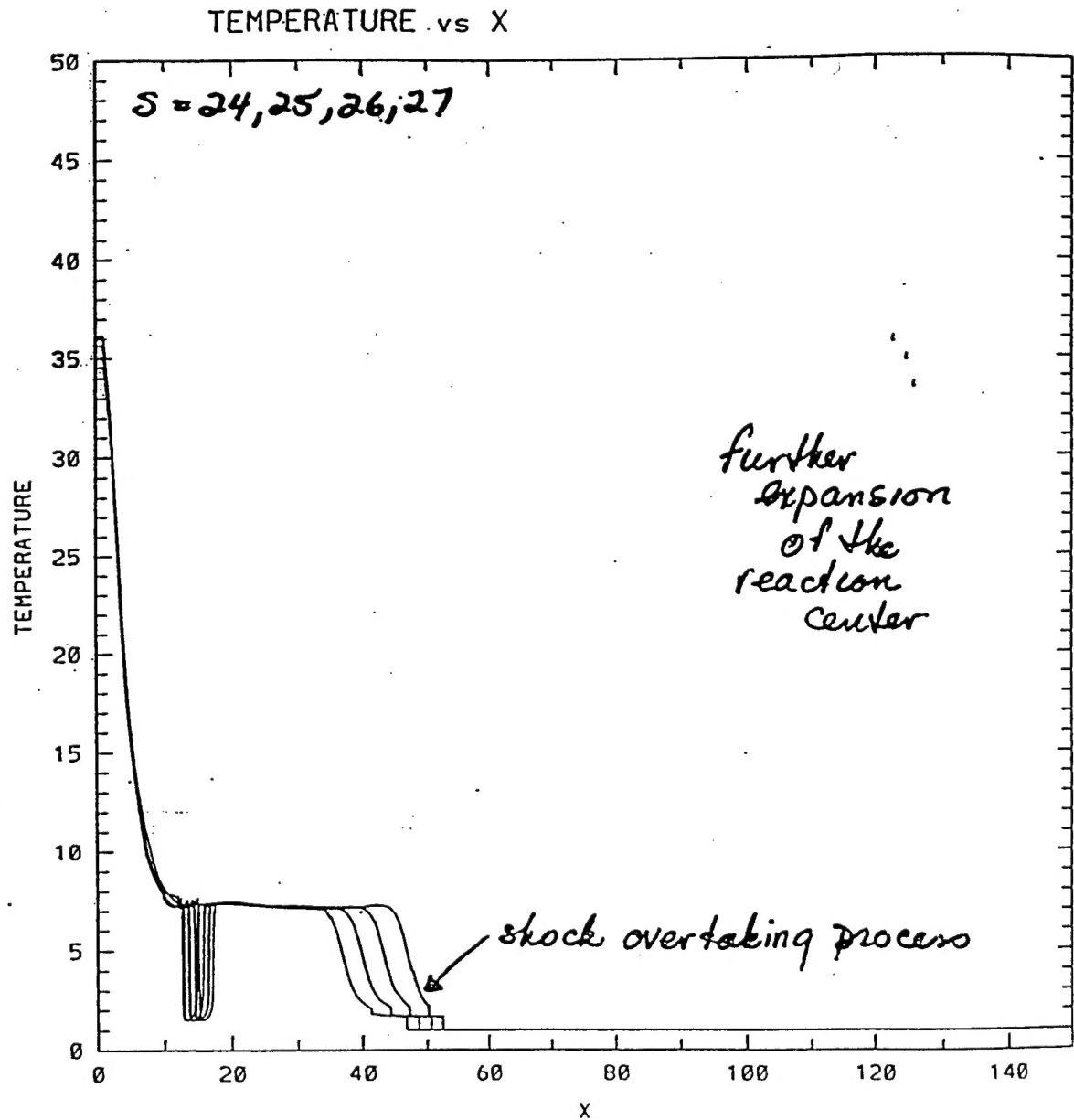
$$\rho(u_t + u u_x) = -p_x/\gamma \quad , \tag{3}$$

$$(\rho C_v/(\gamma - 1))(T_t + u T_x) = -p u_x + \rho \hat{Q} + (\rho \hat{B} q Y/(\gamma - 1)) \exp(-1/\epsilon^* T) \quad , \tag{4}$$

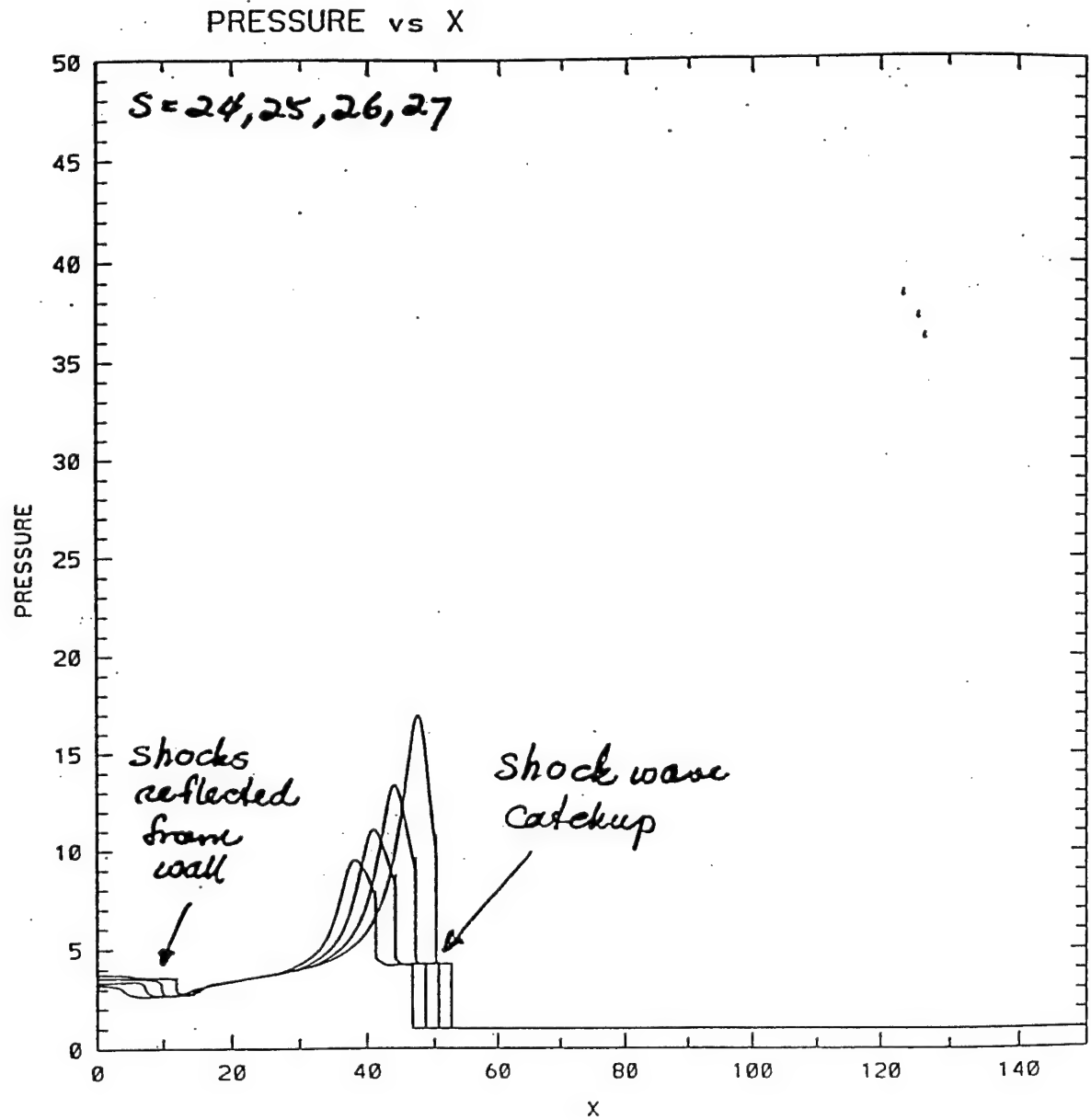$$Y_t + u Y_x = -(\hat{B} Y/\gamma) \exp(-1/\epsilon^* T) \quad , \tag{5}$$

TEMPERATURE vs X

S= 16, 17, 18, 19

cold, unburned mixture

reaction center

B=15.0000 H= 6.0000 EPS= 0.0725 PR= 0.7200 G= 1.4000 DX= 0.0050 CON= 0.9200 T= 16.000

Fig. 1

TEMPERATURE vs X

$S = 24, 25, 26, 27$

further
expansion
of the
reaction
center

shock overtaking process

B=15.0000 H= 6.0000 EPS= 0.0725 PR= 0.7200 G= 1.4000 DX= 0.0050 CON= 0.9200 T= 24.000

Fig. 2

PRESSURE vs X

$S = 24, 25, 26, 27$

shocks
reflected
from
wall

Shock wave
Catehup

B=15.0000 H= 6.0000 EPS= 0.0725 PR= 0.7200 G= 1.4000 DX= 0.0050 CON= 0.9200 T= 24.000

Fig. 3

TEMPERATURE vs X

$S = 28, 29, 80, 31$

Shocks coalesce.

ignition of a third reaction zone
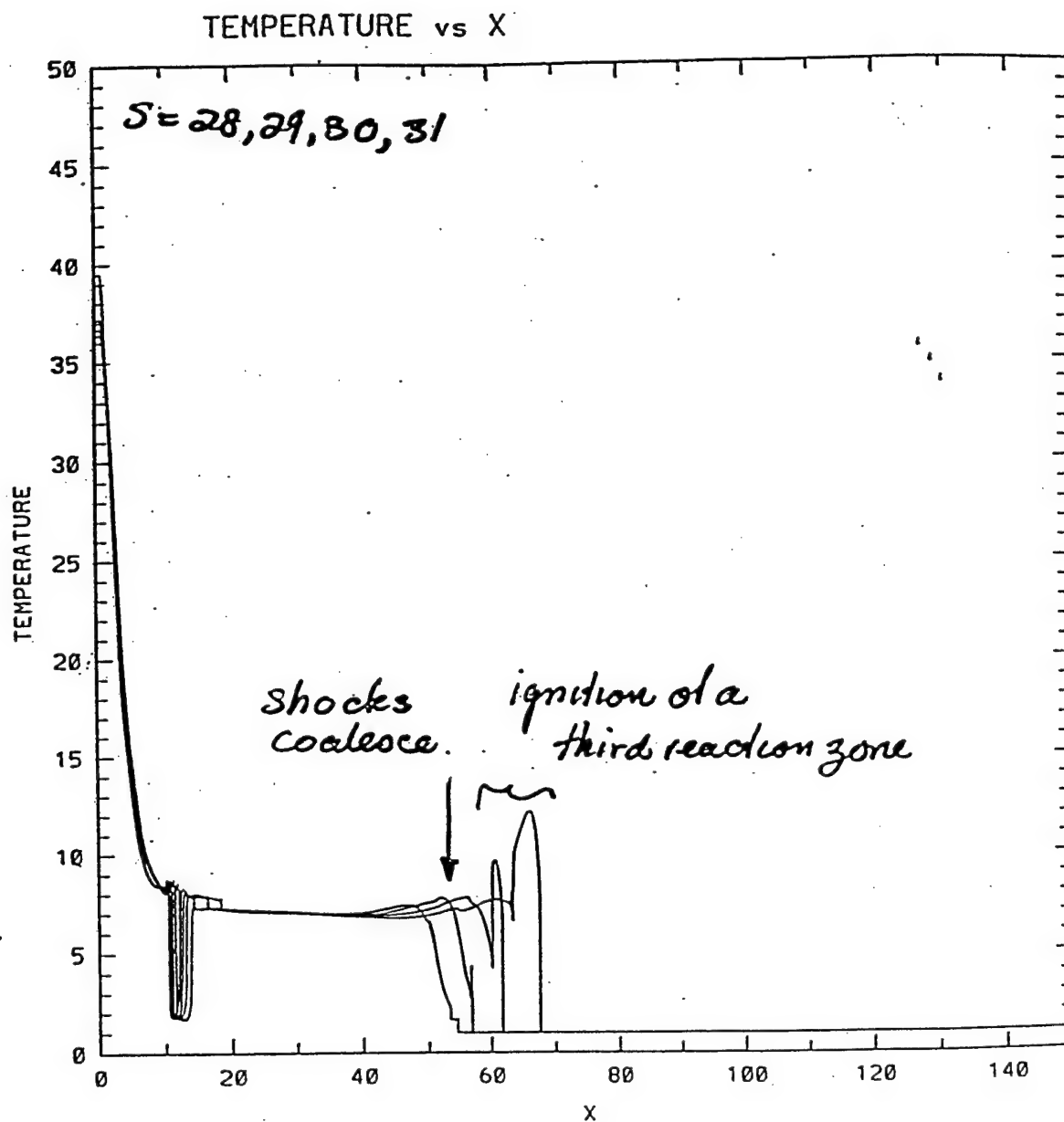
B=15.0000 H= 6.0000 EPS= 0.0725 PR= 0.7200 G= 1.4000 DX= 0.0050 CON= 0.9200 T= 28.000

Fig. 4
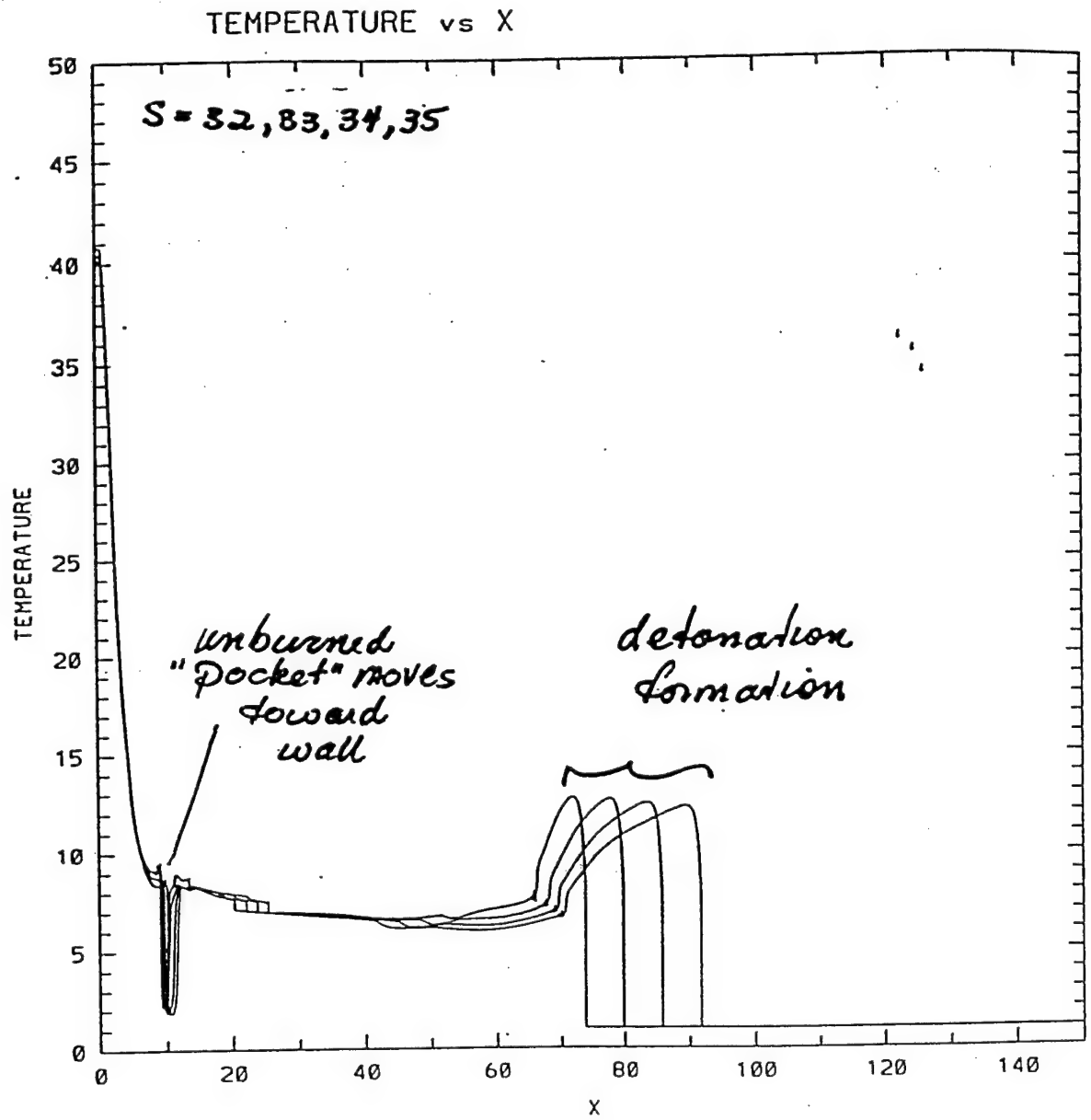
Fig. 5

HEAT ADDITION vs. TIME

Labels on figure: "maximum power burst", "initiating power", "initial "thermal explosion"", "heat release from unburned "pocket""
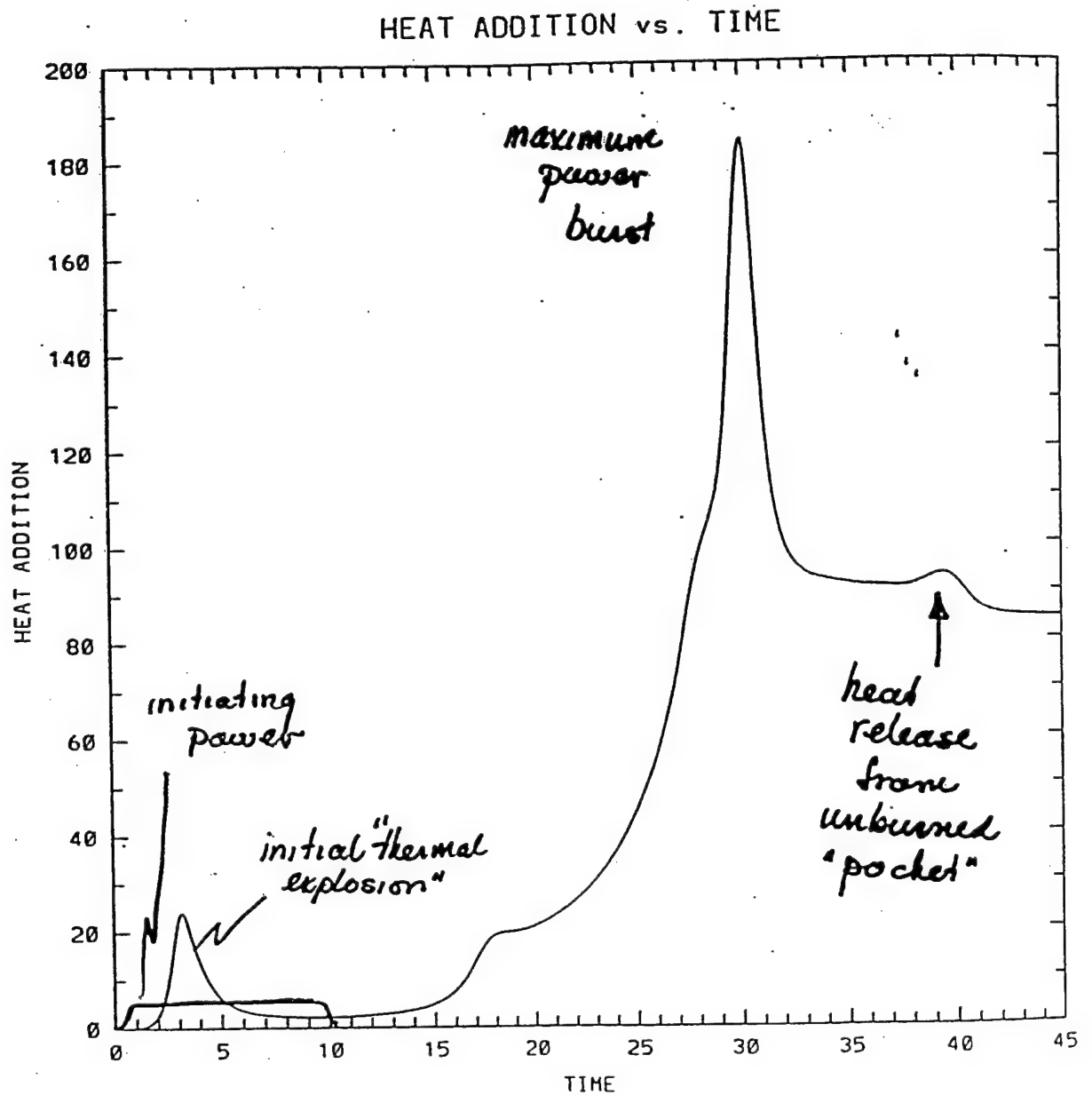
B=15.0000 H= 6.0000 EPS= 0.0725 PR= 0.7200 G= 1.4000 DX= 0.0050 CON= 0.9200 T= 44.991

Fig. 6

The variable Q, defining the thermal power deposition, appears in the lower left corner of Fig. 6. The other quantities have standard definitions, given in (23).

It is notable that these results and those given earlier in Ref. 23, show that the planar detonation formation process, arising from thermal initiation is characterized by irregular, transient processes. Recent work by Eckett et. al. (20) confirms this conclusion for a multidimensional model employing complex kinetics.

These studies of planar processes occurring in a model gaseous reactant mixture, initially at rest, provide an intriguing glimpse of possible detonation creation phenomena. The overriding importance of sequential heat release and wave generation from localized explosions is supported by other theoretical and experimental studies of multidimensional and multiphase systems (examples include Refs. 29 and 30. In addition, the results unify two traditional concepts for DDT found in the literature. The first has DDT resulting from gradients in the induction time (31) while the second focuses on the role of hot spots (32). The sample results presented in Figs. 1-6 provide an integrated view of DDT processes.

Future Opportunities

Mathematical modeling of thermal initiation in the PDE and PDRE environments should be developed in the future. They will provide an opportunity to elucidate the basic physics and chemistry of an initiation event driven by igniter power level, duration and location in an injected, turbulent reactive flow with gaseous and/ liquid components.

The outcomes of this type of mathematical modeling research are to;
1. predict PDE-system parameters needed for successful DDTs, including length and time scales
2. predict criteria for detonation failure in PDEs
3. compare detonation initiation and evolution in models of gaseous and multiphase reactant mixtures
4. predict maximum pressures, endwall pressure time-history, detonation wave speeds, reaction zone lengths, as well as heat transfer and viscous effects in wall boundary layers

These outcomes will be obtained from models based on the complete conservation equations for high speed, reactive gasdynamic flows (33) and reduced forms like those in Eqs.[1]-[5], above. Systematic nondimensionalization, like that used in Refs. 23 and 24 can be used to derive working equation systems that are robust for a wide range of time and length scales. Both, one-, and two-dimensional models for gaseous and multiphase reactant systems can be developed and solved with an effective Flux-Corrected Transport algorithm, described in Ref. (34). Asymptotic methods can be used with the nondimensional equations to describe small scale features evolving on short times scales, like reaction zone structure, hot spot formation and explosion and the concomitant compression wave generation.

(a) Thermal initiation of detonations in gaseous reactants: Given prior experience with modeling planar initiation, it is easy to be quite explicit about the scenario for this

research effort. The mathematical model describes the spatially resolved time-history of detonation formation arising from thermal power deposition in a PDE environment. Initially, hot products of reaction from the previous cycle are present in the chamber at a specified backpressure, compatible with the altitude and configuration of the operating PDE. Volumetric heat addition, representing the impact of a spark igniter, occurs subsequent to injection of a reactive gas mixture from the endwall. As a result, the combustion initiation process occurs in a moving gas. A range of power deposition (igniter) location, relative to the injection location, power level and firing duration are considered. Initially, simple, exothermic, one-step kinetics model chemical effects in order to focus on the impact of localized heat addition on the reactive gasdynamic transients. The activation energy and reaction times are available as additional parameters. More elaborate reduced kinetics can be used subsequently.

The spatial distributions of pressure, density, temperature, reactant consumption and heat release as functions of time are to be found, in analogy with the results given in Figs. 1-6. These results can be used to construct a comprehensive description of the detonation birth process and propagation through the PDE chamber to the interface region between the reactive mixture, the buffer gas and the hot products of the reaction beyond. In addition, the initiation shock, the interface, each of the compression waves arising from rapid heating of reaction centers and the coalescence of waves leading to detonation formation can be tracked in space and time. The ensemble of results can be used to predict the sensitivity of the endwall pressure, $p_e(t)$, to the aforementioned parameters. In particular, a time-averaged endwall pressure, optimized for fuel consumption will provide a PDE efficiency criteria.

The computational calculation is done in the PDE context, as opposed to the detonation tube environment (e.g., (23), (24) and (35)). A reactant filling phase is considered first. The mass addition pulse from the injectors initiates a lead shock that propagates through the hot gas products remaining from the previous cycle. The interface separating the fresh reactants from the products[1] follows at a lower speed commensurate with the injection process. The shock front is tracked to the PDE exit, at which time the one-dimensional computation is terminated.

Prior to the time at which the initiation shock reaches the exit, a prescribed thermal power is deposited into a compact volume (at specified grid points) for a limited time period. This provides a specific initiation energy density (J/m^3). The deposition region is either adjacent to the endwall or separated by a specified downstream distance. Localized gas heating initiates a rapid reaction event that is the source of compression waves. In the case of deposition adjacent to the endwall, waves propagating toward the exit initiate a complex sequence of localized exothermic events that lead to the appearance of a detonation. Solutions describe the impact of power deposition level and duration, as well as, kinetic parameters, on the formation process and the DDT length.
When the heating occurs at some distance from the endwall there is an opportunity for backward moving compression waves to heat the reactive material twice: once while moving toward the endwall and then again after wave reflection occurs (see Ref. 29 for a related example). The resulting delayed explosion is the source of a new set of

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[1] Initially, the buffer gas, used to reduce premature ignition, is neglected.

compression waves which run forward through relatively hot gases previously processed by the initial wave set. It is anticipated that the detonation formation process can be accelerated by these late arriving waves, an effect seen in multiphase detonation formation (11, 12). Our studies of this configuration seek to determine if optimized combinations of igniter location, level and duration of power deposition can accelerate the formation of a strongly driven detonation. Short DDT lengths will enable a fully developed detonation to process a relatively larger amount of injected mixture. The numerical results are used to track the various shocks, the propagating combustion zones and their coalescence. In addition the endwall pressure time history is obtained for use in the thrust calculation.

The timing sequence for filling, ignition and detonation formation processes in the planar model is designed to enable the detonation to reach the fresh mixture-burned gas interface before the lead shock reaches the exit of the PDE chamber. This is done to avoid modeling the multidimensional expansion wave processes near the exit, subsequent to shock passage across the exit plane (14).

b. Thermal initiation of detonations in multiphase reactants: This more challenging phase of the research project is focused on modeling transient reactive gasdynamics in sprays composed initially of one gas phase and one liquid phase. Initially, the focus can be on low volatility hydrocarbon droplets (e.g., JP-10) in air or oxygen. Subsequently, a model for liquid oxygen droplets in a gaseous hydrogen environment will be considered (36). These condensed phase propellants are advantageous in PDE and PDRE applications where storage issues are important for mission effectiveness.

While much has been done with spray combustion in the quasi-steady environment (37), the effort to model basically transient processes associated with detonation initiation is less developed (38-40). The primary challenge here is to develop a physically accurate model for the interaction of droplets with a gaseous environment undergoing significant pressure and temperature transients due to localized power deposition from an igniter or from local exothermic chemistry, and/or from the passage of strong compression and shock waves. Fortunately, there is a significant experimental and theoretical data base for detonation initiation in low volatility fuels.

Refs. 5, 26, 27, 41 and 42, among others, provide considerable insight into the physical processes involved in the blast wave initiation of detonations and quasi-detonations in low volatility droplet sprays. In addition, experimental PDE operations based on JP-10 fuel have been described in Refs. 11 and 12. A summary, given in Ref. 52b, is available from the author of this report.

Detonation initiation in low volatility droplet sprays differs considerably from that in premixed gaseous systems. Droplets must be "processed" by the transient high-speed flow field in order to prepare a combustible fuel/oxidizer mixture. A droplet intersected by a shock is heated, deformed and accelerated. The droplet velocity lags the gas velocity to the extent that there is a locally supersonic flow around the droplet. A bow shock is wrapped around the droplet. Shear stresses strip small drops of liquid from the surface of the primary droplet, resulting in a micromist wake downstream. The micromist wake, accelerated by local drag forces (due to relative velocity with the gas)

much faster than the primary droplet, is elongated with time and likely to be turbulent. Meanwhile, the bow shock wrapped around the droplet surface causes significant heating of the local stagnation point along with vaporization and mixing. Localized ignition can occur near the stagnation point. Burning gases are convected around the droplet, through a wake shock and into the micromist. Under appropriate conditions the mist mixture explodes on a very short time scale, sending pressure waves toward the lead shock. It is strengthened by coalescence and can then process additional intersected droplets more quickly. If the appropriate feedback process occurs, the combustion wave is driven into a detonation mode, in that the lead shock propagation is supported by heat release from a reaction zone of considerable length (cm. length scales are common), relative to that found in a premixed gaseous system.

Gas-phase detonations with extended reaction zones tend to fail because the lead shock has little support from the quasi-steady exothermic processes occurring downstream. In contrast, spray detonations with extended reaction zones can prevail because the sequence of transient explosions from the wake of each droplet creates a compression wave system that can propagate up to, and support the lead wave. This suggests an analogy with the impact of the localized transients, seen in Figs. 1-6, on detonation initiation. It is the rapid transient character of the micromist explosion that enables the spray detonation to evolve.

Generally, spray detonation initiation and evolution are facilitated by smaller droplets, an oxygen, as opposed to air, environment and appropriate equivalence ratios (5). Detonation wave speed deficits, relative to analogous C.J.-values, decrease as the drop size is reduced. Brophy and Netzer (12), have taken advantage of this fact to use JP-10 droplets with Sauter Mean Diameters between 6 and 10 μm to operate a model PDE at frequencies up to 10hz.

Data from the aforementioned and related experiments can be used to develop a physically viable model for droplet "processing" in a detonation environment. Key time scales can be integrated into the model, with the objective of describing the consequences of sequential explosions in isolated volumes of micromist. This type of model, incorporating more transient spray physics than seen in Refs. 38-40, should enable a more accurate prediction of the spatially distributed exothermic transients (effective chemical induction times), and the associated transient compression systems needed to support the detonation.

Here again, the focus is on thermal initiation, similar to that used in Refs. 11 and 12, rather than the more commonly used blast wave initiator (5, 26,27, 40-42). A model can be developed for localized power deposition into a recently injected spray with a specified equivalence ratio, a key parameter in spray detonations (12). The initial goal should be to describe how the heating and gasdynamics of the igniter initiate rapid transient combustion in the spray cloud. The reduced chemistry models for JP-10, described by Li et. al. (43), can be used to assure realistic chemical time scales and kinetic parameters. Initially, the planar model can be used to generate a spray analogue for results described in Figs. 1-6, above. An early objective is to capture the sequential exothermic events that appear to characterize successful detonation initiation in sprays (5). A second objective is to predict the effect of igniter characteristics on the

detonation initiation process. In particular, it is of interest to find the minimum energy requirements for reliable, repetitive operation, specific to the reactant mixture and geometrical configuration employed. Additionally, the endwall pressure transient can be predicted and used to find the specific impulse during reactive portion of the PDE cycle. This value may differ from that found in gaseous detonations because unburned reactants far behind the lead combustion wave system can continue to burn for extended periods. Comparisons with analogous gaseous system results for wave speeds and maximum pressures will provide a measure of the relative effectiveness of multiphase PDE operation.

Coy and Levine (36) have proposed the use of liquid oxygen droplet-hydrogen gas sprays for PDRE's. This spray will have very different combustion characteristics from those discussed previously. In, particular, the drops will be heated and easily vaporized in an hot operational environment. The flash evaporation of a high density of oxygen droplets can generate a significant boost in the endwall pressure prior to detonation initiation. The combination of the evaporative pressure rise and that due to subsequent combustion may generate a desirable endwall pressure transient and associated specific impulse. Experimental results for detonations in liquid oxygen droplet/hydrogen gas sprays do not appear to be available in the literature. It is anticipated that Coy and Levine (36) will develop an experimental capability in the next 12 months. They plan to assess droplet behavior in a gasdynamic environment, including deformation, shattering due to shock wave interactions and combustion of residual droplets far behind the wave. Measurements will be made of critical initiation energies for a variety of wave and thermal igniters, reaction zone lengths and pressure transients. Modeling of experiments can be done in cooperation with the Air Force group to predict peak pressures, wave speeds, reaction zone lengths, DDT lengths, thermal losses to the detonation tube wall viscous losses in the boundary layer.

2b. Secondary Objective-SRM Modeling

A summary of each manuscript developed during the grant period and/or relevant publications are described in the following paragraphs.

Zhao et. al (44) formulate an initial-boundary value problem to describe a weakly nonlinear theory for the evolution of flow disturbances arising from prescribed transient axial velocity disturbances on the endwall of a cylinder with uniform sidewall injection. The model is valid for large axial Reynolds number (Re), small axial Mach number (M) and a large aspect ratio cylinder (δ). A small but finite acoustic field driven by the transient boundary condition interacts inviscidly with the fluid injected from the sidewall to create intense transient vorticity on the boundary. Nonlinear convection-diffusion equations describe the physical processes that distribute the boundary-generated vorticity into the cylinder. When the injection rate is sufficiently small, the vorticity in always confined to a boundary layer adjacent to injection surface which is thicker than a tradition acoustic boundary layer. However, for larger values of injection a different scenario plays out. For sufficiently small values of time the intense transient vorticity is locate adjacent to the injection surface in a gradually thickening layer with a clearly defined edge. Eventually, the vorticity fills the entire cylinder. This formulation avoids the inherent limitations of a linear stability analysis with assumed, rather than calculated, infinitesimal,

quasi-steady pressure disturbances. The current nonlinear formulation can handle pressure variations as large as about 10% of the baseline value, far larger than the 0.1% permitted in a linear theory.

Azimuthally-dependent propellant burning transients are simulated by Staab and Kassoy (45) by imposing a transient sidewall injection rate that varies with the angular variable θ as well as with time and axial location. Both standing and traveling wave injection distributions w/r to the azimuthal coordinate can be imposed on the interior circumference of the cylinder. Solutions for standing wave sidewall disturbances show that only axial, planar acoustic waves are driven in a large aspect ratio cylinder. However, there is also a non-acoustic time-dependent three-dimensional flow induced in the chamber. Non-axisymmetric cross-sectional flow is described with a non-zero velocity across the axis of the cylinder.

The vorticity components (azimuthal and axial) are generated on the sidewall by inviscid interactions between the transient pressure gradients (axial and azimuthal) and the fluid injected from the sidewall. This implies that the sidewall wall will be "scoured" by a transient azimuthal shear stress in addition to the previously discussed axial shear stress. The subsequent distribution of the vorticity in the cylinder is described by nonlinear convection-diffusion equations for the disturbance amplitudes considered in our model. The time dependent distribution process is shown pictorially in Ref.2, which includes instantaneous azimuthal velocity profiles on a cylinder cross-section.

The non-axisymmetric vorticity front shape can be calculated from first principles as part of the analysis. Instantaneous vorticity distribution results are given for two different distributions of the azimuthally dependent injection rate. Solutions show that for times large compared to the axial acoustic time in the chamber, the front shape approaches an axisymmetric configuration. The amplitude of the vorticity in the chamber is maximized at azimuthal coordinate locations where the local injection rate is largest. This implies that a local zone of intense propellant burning can be the source of intense vorticity, independent of the turbulence properties of the flow field.

The three-dimensional modeling, based on asymptotic methodologies, has been developed in part to by-pass the effort needed to construct large complex codes for studying transient multidimensional processes in a motor chamber.

Kirkkopru et.al (46) revisit a computational model for flow induced in a cylinder by uniform sidewall injection when a prescribed pressure gradient is present at the exit plane. Grid resolution is improved by using the radial scaling derived from previously mentioned asymptotic studies. A careful analysis of the data shows that the acoustic field predicted by the computation contains primarily the standing wave response to the disturbance at the exit plane. In fact there is excellent quantitative agreement between the analytically predicted standing wave distribution and that found from computational results. However, the sustained traveling wave response (eigenfunctions) predicted by the analysis appears in the computation only for very short times and is rapidly damped away. The present numerical method, including the boundary condition approach is not able to capture eigenfunctions, probably because wave reflections are not adequately

treated at boundaries. This deficiency is true for all other similar computations carried out in the past. A remedy is given in Refs. 47 and 48, discussed below.

Although the acoustic pressure distribution is not totally accurate one can make quite reasonably comparisons of the rotational axial velocity distribution in the cylinder found computationally and quasi-analytically. In fact the deviations are most pronounced adjacent to the injection surface and increasingly smaller as one moves radially toward the cylinder axis. This outcome is reasonable because the pressure field determines how vorticity is generated at the injection surface, while the subsequent evolution of that vorticity is determined by a nonlinear balance of convection and viscous diffusion. The latter is a likely source of eigenfunction-effect damping.

By driving the co-existing acoustic and rotational flow transients with explicit boundary disturbances, we establish a clear cause and effect relationship between the transient internal flow dynamics and the imposed conditions on the endwall or sidewall. Forcing on the latter boundary is particularly relevant to simulating unsteady propellant burning. Our numerical simulation involves fewer assumptions than those needed in more traditional turbulence modeling (e.g., closure models), and may provide considerable insights into the transient dynamics of weakly viscous, low Mach number, compressible flows with co-existing acoustics and vorticity.

An understanding of oscillatory, intense axial shear stress on the sidewall will be useful for developing physically viable boundary conditions at the decomposing interface of a burning solid propellant. The idea here is account for the "scouring" effect of oscillatory shear stress on the fizz-foam zone thought to exist at the gas-propellant interface. Although the axial velocity in the combustion zone may be small, the results of our nearly isothermal flow studies suggest that the velocity gradient will be relatively large, and hence can be a source of axial deformation, and perhaps stripping of easily deformable surface material.

A full numerical simulation of the transient flow response to prescribed boundary disturbances is given by Hegab and Kassoy (47,48) with a particular focus on the thermal properties of the internal flow in a channel with time-dependent sidewall mass addition.

The computed axial velocity is divided into three parts. The steady field is valid for a constant injection velocity. An acoustic disturbance, driven by an additional transient injection velocity component, is composed of standing and traveling waves. Finally, the rotational velocity distribution, driven by the presence of the acoustic field, is used to describe the intense transient vorticity disturbances. Temperature variations driven by small acoustic disturbances are captured along with surprisingly large radial temperature gradients that fill the entire channel flow field.

The temperature distributions show that the small but finite amplitude planar acoustic field co-exists with a temperature distribution that has significant radial gradients. As a result, the heat transfer at the injection surface is considerably larger than that expected from the acoustic temperature disturbances alone. These results are entirely compatible with the theoretical predictions in Refs. 44,45, 49 and 50.

Results are presented in Refs. 47 and 48 for increasingly detailed axial injection distributions in a channel. The resulting spatial distribution of vorticity in the chamber is found to have an increasingly complex spatial morphology with respect to radial and axial variations. Significant cellular structures are present when the axial wave number of the injection distribution is sufficiently large. This suggests the possibility of high wave number (small length scale) vorticity in the chamber arising from deterministic processes of the kind discovered in the quasi-analytical studies rather than from the more familiar hydrodynamical instabilities associated with turbulence.

The numerical data has also been analyzed in terms of mean flow and fluctuating flow properties to show how the presence of co-existing rotational and acoustic disturbance alter the more familiar patterns for turbulent injected channel flows without acoustics.

A comparison of the mean flow and instantaneous axial velocity profiles at specific parameter values shows that the former does not hint at the spatial variations of the axial velocity shown in the latter. In particular, the relatively large wall shear stress in the instantaneous profile (which varies in time between positive and negative values) is not reflected in the mean flow value. The latter alone, may not be a useful measure of the "scouring" effect arising from a time dependent, rapidly varying wall shear stress on the fizz-foam surface layer of a decomposing solid propellant.
The RMS intensity distribution in a channel includes the effects of both the rotational and acoustic transients, as mentioned above. One notes several local peaks across the radius, with the largest value near the sidewall. In general, the amplitude increases, and the local peaks move toward the sidewall with increasing axial distance downstream. The multiple peaks arise from vorticity generation driven by axial acoustic waves in the cylinder

Rempe et. al (49,50) describes an asymptotic analysis of the thermal processes occurring in the nearly isothermal cylinder flow. Although the temperature variations associated with acoustic phenomena are small, O(M), one finds that O(1) sidewall heat transfer is encountered. The analysis explains how these unexpectedly large radial gradients arise. A linear convection-conduction equation for the temperature distribution describes the evolution of the thermal processes in the cylinder. Numerical solutions for the temperature field are obtained for time values up to 60 axial acoustic times. To our knowledge, no other researchers have predicted the large wall heat transfer found in our studies nor the evolution of the spatially distributed temperature.

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52. *Unpublished Reports:*

a. Jennifer Russell, "An Introduction to Detonation Waves and Pulse Detonation Engines" Independent Study Final Report, Mechanical Engineering Department, University of Colorado, May 1, 2000

b. Tanarit Sakulyanontvittaya, "Literature Review of Experiments Involving Detonations in Liquid Fuel Spray/Oxidizer Mixtures", Final Report for Introduction to Research, MCEN 5208

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- **D. R. Kassoy** is a Professor of Mechanical Engineering at the University of Colorado at Boulder. He is the author of more than 95 published papers. Much of his recent work has focused on the modeling of low and high speed reactive systems, including flames, combustion, detonations and explosions, as well as acoustic-vorticity dynamics in rocket motor chambers. Kassoy has been the recipient of a Guggenheim Fellowship, a Fulbright Research Award, a Fellowship from the Japan Society for the Promotion of Science, and is a Fellow of the American Physical Society (Division of Fluid Dynamics

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- **Kadir Kirkkopru** is a Professor of Mechanical Engineering at the Istanbul Technical University in Turkey. He has been a Research Associate at the University of Colorado at various times throughout the past ten years. Currently, he shares a NATO Cooperative Research Grant with D.R. Kassoy on the topic of rocket motor fluid dynamics and combustion

5. PUBLICATIONS AND APPENDICES (cover page and/or abstract only)

a. J. A. Kuehn, D. R. Kassoy, J. F. Clarke and N. Riley, "The Origin and Evolution of a Planar Detonation Following Thermal Power Deposition in a Reactive Gas", work in progress, (2001)

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The Origin and Evolution of a

Planar Detonation Following Thermal

Power Deposition in a Reactive Gas

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Acoustically generated vorticity in an internal flow

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A mathematical model is formulated to describe the initiation and evolution of intense unsteady vorticity in a low Mach number (M), weakly viscous internal flow sustained by mass addition through the sidewall of a long, narrow cylinder. An $O(M)$ axial acoustic velocity disturbance, generated by a prescribed harmonic transient endwall velocity, interacts with the basically inviscid rotational steady injected flow to generate time-dependent vorticity at the sidewall. The steady radial velocity component convects the vorticity into the flow. The axial velocity associated with the vorticity field varies across the cylinder radius and in particular has an instantaneous oscillatory spatial distribution with a characteristic wavelength $O(M)$ smaller than the radius. Weak viscous effects cause the vorticity to diffuse on the small radial length scale as it is convected from the wall toward the axis. The magnitude of the transient vorticity field is larger by $O(M^{-1})$ than that in the steady flow.

An initial-boundary-value formulation is employed to find nonlinear unsteady solutions when a pressure node exists at the downstream exit of the cylinder. The complete velocity consists of a superposition of the steady flow, an acoustic (irrotational) field and the rotational component, all of the same magnitude.

1. Introduction

Intense transient vorticity can be generated in a tubular internal flow by an interaction between a forced acoustic field and fluid injected normally from the cylinder sidewall. This occurs at a given axial location because the transient axial gradient of the acoustic pressure drives time-dependent wall shear stress variations. The resulting radial gradient of the axial velocity is convected into the cylinder by the injected flow field. As a result, one finds co-existing irrotational and rotational disturbances of the same magnitude.

The spatial distribution and time-history of the vorticity depend upon the characteristic amplitude of the wall injection speed (V_{r0}'), the length (L') and radius (R') of the cylinder, the frequency of the acoustic forcing (ω'), and the fluid properties. It follows that the crucial non-dimensional parameters include, the flow Reynolds

Thermal Response for an Internal Flow in a
Cylinder with Time Dependent Sidewall
Mass Addition

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38th Aerospace Sciences
Meeting & Exhibit
10-13 January 2000 / Reno, NV

Three-dimensional Flow in a Cylinder with Sidewall Mass Addition

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March 9, 2000

Abstract

Three-dimensional, time-dependent, nonlinear flow dynamics within a cylinder with sidewall mass injection are investigated. A non-axisymmetric transient injection velocity, prescribed along the sidewall boundary of a long, narrow, half-open cylinder, induces a low Mach number, high Reynolds number flow. The injection drives nearly planar axial acoustic disturbances, which interact with the injected fluid to produce the azimuthal component of vorticity on the sidewall in an inviscid manner. A smaller, but important azimuthally-dependent transient disturbance, driven by the non-axisymmetric injection disturbance leads to the axial component of vorticity on the cylinder sidewall. Both components of vorticity are shown to convect toward the center of the cylinder, diffuse radially, and convect downstream. Other results show that the axial component of vorticity produced along the sidewall is largest near the maximum of a mass source distribution in the azimuthal dimension. The amplitude of the axial vorticity component decreases significantly away from the injection surface and at other azimuthal locations. The analysis of these flow processes is based on the full three-dimensional Navier-Stokes equations. Limit processes based on the behavior of the axial Mach number $M \to 0$, are used to derive reduced equations. It is shown that the primary rotational flow response is described by a nonlinear, convection-diffusion equation.

1   Introduction

Time-dependent three-dimensional internal flow dynamics in a cylinder with mass injection are studied with a goal of understanding the generation and evolution of vorticity within the cylinder. Mass is injected non-axisymmetrically along the sidewall of a cylinder with one open end, and the time-dependent injection generates nearly axially-planar acoustic pressure waves which interacts with the fluid injected from the sidewall to generate vorticity on the boundary. The axial gradient of the pressure interacts with the injected fluid to produce azimuthal vorticity of magnitude proportional to the inverse Mach number, while the smaller-magnitude azimuthal pressure field interacts with the injected fluid to produce order-one axial vorticity. The

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Internal Flow Temperature Dynamics in a Channel with Time-dependent Mass Injection

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Abstract

Most of the recent studies of chamber flow dynamics in models of Solid Rocket Motors (SRM's) provide the spatial distribution of the transient velocity and vorticity without any consideration of the accompanying temperature response. In this paper, the transient co-existing acoustic-rotational flow dynamics generated in a chamber with time-dependent mass injection is studied with the goal of understanding the accompanying heat transfer and temperature dynamics throughout the system. The compressible Navier-Stokes equations are solved computationally. Boundary conditions on the sidewalls and the exit plane are written in Navier-Stokes characterstics form in order to retain proper wave reflection processes. Transient solutions consist of coexisting, equal magnitude acoustics (irrotational) and vorticity as well as surprisingly large transverse temperature gradients across the chamber. The computational results for low Mach and large Reynolds number chamber flow show that large transient temperature gradients are transported from the wall into the chamber by the transverse velocity component of the flow field. Large gradients at the sidewall imply that the associated heat transfer may influence the

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combustion zone above a burning propellant. Results for a near-resonant frequency of the time-dependent injected fluid show that the maximum spatial temperature oscillations are about ten times greater than that for non-resonant frequencies. The time-dependent numerical data is also used to calculate the mean axial velocity distribution across the chamber and RMS values for the velocity and vorticity fields to observe the characteristics of a flow field with co-existing acoustics and vorticity.

Introduction

Time-dependent, compressible fluid dynamics in a planar slot resulting from low Mach number, transient sidewall mass injection are studied computationally to ascertain thermal properties of the flow and heat transfer to the boundaries. The axially distributed transverse velocity on the sidewall is a prescribed function of time and the temperature of the injected gas is specified. This work extends that of Kirkkopru et. al.[1,2] who study the velocity and the vorticity fields in a cylinder with one open end and similar sidewall boundary conditions, but do not consider thermal effects. The results of the present study show that surprisingly large transient temperature gradients are present on the sidewalls and in the interior of the channel, even when the transverse fluid injection is isothermal. This unexpected phenomenon arises from an interesting interaction between acoustic disturbances present in the low Mach number internal flow and the isothermal fluid injected from the boundary.

Staab et al.[3], Rempe et al.[4] and Zhao et al.[5] employ asymptotic methods to demonstrate that unsteady addition of mass from the lateral boundaries of a cylinder is the immediate source of acoustic disturbances that propagate in the low axial Mach number (M), high Reynolds number (Re) mean flow. Their analytical results are used to prove

An Introduction to Detonation Waves and Pulse Detonation Engines

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Thermal Response for an Internal Flow in a Cylinder with Time Dependent Sidewall Mass Addition

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December 14, 2000

1   Introduction

Time-dependent internal flow dynamics in a cylinder with one open end are studied with a goal of understanding the associated heat transfer and temperature dynamics. The transients are cause by mass injected from the cylinder sidewall with a prescribed unsteady axial distribution and a specified constant temperature. This work extends that of Staab et al.[16], who study only the vorticity and velocity fields within a cylinder with the same sidewall boundary condition. The current work shows that the small acoustic temperature disturbance interacts with the constant temperature injected fluid to generate unexpectedly large temperature gradients at the sidewall. These gradients are then convected toward the centerline and downstream and diffused radially. The results provide a better understanding of the temperature response of the fluid within a simplified version of a solid-fuel rocket motor (SRM) chamber. In particular, the sidewall boundary condition models the normal velocity of gaseous products formed by the combustion of propellant.

The work of Staab et al.[16] shows that in an asymptotic analysis for small axial Mach number, M, the equations that describe the velocity field can be decoupled from those describing the temperature field and only velocity and vorticity dynamics are studied in that work. The current work is devoted to finding solutions to the latter so that energy dynamics, and especially the temperature and density fields are known to $O(M)$. Zhao et al.[20] show that the largest part of the transient energy disturbance in a cylinder with sidewall mass addition arises from the $O(M)$-temperature field. The leading-order energy fluctuations are proportional to the leading-order temperature field, on the order of the Mach number. In comparison, the kinetic energy variation is $O(M^2)$.

The current work incorporates an integral scaling transformation developed by Zhao and Kassoy [19] and described more recently by Zhao et al.[20] in place of the simple linear scaling transformation for the radial variable used in Staab et al.[16]. Use of the former radial transformation results

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AN INTRODUCTION TO DETONATION WAVES AND PULSE DETONATION ENGINES

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ABSTRACT

This paper provides an overview of detonation waves and the application to Pulse Detonation Engines (PDEs). First, a discussion of detonation waves furnishes a survey of the basic physics of a detonation wave and explains detonation initiation. Then, a demonstration of PDE operation is given, including a comparison of air-breathing and rocket engines. Finally, a review of the research performed in experimentation and modeling of PDEs is given.

INTRODUCTION

Deflagration, explosion, and detonation waves are all results of large amounts of energy that are suddenly released due to chemical reactions. Deflagration is the most common type of combustion. A deflagration reaction propagates at relatively low speeds, usually on the order of one or more meters per second for typical hydrocarbon/air mixtures. The speed is limited by the amount of heat released. Deflagrations can be modeled as constant pressure processes. In contrast, detonations are modeled as constant volume processes. Detonations are supersonic combustion waves that propagate and a few thousand meters per second. Clearly a detonation is more energetic than deflagration and thus produces higher pressures and temperatures. The difference between explosion waves and detonation waves lies in the time in which energy is released. Explosion waves are 2-4 orders of magnitude slower than detonation waves[1]. A detonation wave is a composite wave consisting of a shock wave sustained by the chemical energy released in the flame zone immediately following the shock front.

1.0 STATE EQUATIONS

The problem of detonation is treated as simple heating, in which the speed of propagation of the wave and the change in properties across the wave are to be determined. Figure 1 shows a schematic of a detonation wave.

unburned gas → ρ_1, p_1, T_1, u_1 | → ρ_2, p_2, T_2, u_2 burned gas
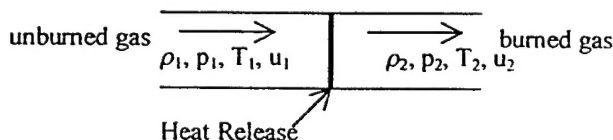
Heat Release

Figure 1: Propagation of a detonation wave.

Analysis of detonation waves is based on the conservation equations for mass, momentum, and energy across the detonation:

mass: $\rho_1 u_1 = \rho_2 u_2$

momentum: $p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2$

energy: $C_p T_1 + (1/2)u_1^2 + Q = C_p T_2 + (1/2)u_2^2$

where

1 refers to the state of unburned gas (upstream of the detonation wave)
2 refers to the state of the burned gas (immediately downstream of detonation)

1

Final report

Literature review of experiments involving detonations in liquid fuel spray/oxidizer mixtures

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Introduction to Research, MCEN 5207, Spring 2001
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Objective: To understand the processes and characteristics of detonations in liquid fuel spray/oxidizer mixtures used in pulsed detonation engine.

Abstract

The Pulsed Detonation Engine (PDE) is a new evolutionary form of a modern propulsion system. While some engines use a reactive gas mixture, the propagation of a detonation through a liquid fuel/oxidizer may produce relatively high thrust levels for system weight. In this literature review, nine articles about experiments in liquid fuel spray detonation are evaluated. First, the principles of PDE and the physics of detonation waves are summarized. Next, experimental methods used in each study are presented. Then the major results in each selected article are integrated and presented in six sections; initiation of detonation, propagation phenomena, effect of droplet size, propagation properties of detonation waves, effect of wall temperature, and optimization of the PDE. These results contain experimental data and other information that will be useful for PDE development. This literature review is preliminary to more advanced studies of experimentation with liquid fuel spray detonation for PDE.

AIAA 2001-0338
The Thermal Response of an Internal Flow in a Solid Rocket Motor Chamber/Nozzle Model

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39th AIAA Aerospace Sciences Meeting & Exhibit
8-11 January 2001 / Reno, NV

Acoustically generated unsteady vorticity field in a long narrow cylinder with sidewall injection

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